Position paper



Digitalisation Task Force

April 2024



ACKNOWLEDGEMENT



Batteries Europe Secretariat is an EU-funded project that has received funding from the European Union's Horizon Europe Research and Innovation Programme under Grant Agreement N. 101069676.

DISCLAIMER

The sole responsibility for the content of this report lies with the authors. It does not necessarily reflect the opinion of the European Union. The European Commission is not responsible for any use that may be made of the information contained therein.

While this publication has been prepared with care, the authors and their employers provide no warranty with regards to the content and shall not be liable for any direct, incidental or consequential damages that may result from the use of the information or the data contained therein.



Batteries Europe Task Force Digitalisation

Chair:	Maher Chebbo (Univers)
Co-Chair:	Simon Stier (Fraunhofer Institute for Silicate Research ISC)
Technical	Christoph Grzeschik (VDI/VDE-IT)
coordinator:	
Lead authors:	António Martins (FEUP - Faculty of Engineering - University of Porto), Edoardo Gino Macchi (Fondazione Bruno Kessler), Elixabete Ayerbe (CIDETEC Energy Storage), Javier Carrasco (CIC energiGUNE), Maher Chebbo (Univers), Mattia Felice Palermo (CIC energiGUNE), Mohsen Shiea (Fondazione Bruno Kessler), Simon Stier (Fraunhofer Institute for Silicate Research ISC), Teresa Mata (INEGI - Institute of Science and Innovation in Mechanical and Industrial Engineering)
Contributing	Alfonso Bello (Eurecat)
authors:	
Task Force	Aitor Apraiz (Mondragon Assembly S.Coop), Alan Pastorelli (Flash Battery),
members:	Aleksandra Kronberga (European Commission), Aleksandra Naumann (Technische Universität Braunschweig), Alain Vassart (Arcadis), Alessandro Romanello (InnoEnergy), Anssi Laukkanen (VTT Technical Research Centre of Finland Ltd), António Martins (Faculty of Engineering - University of Porto), Ari Hentunen (VTT Technical Research Centre of Finland Ltd), Ákos Dervalics (InnoEnergy), Christophe Grzeschik (VDI/VDE-IT), Edoardo Gino Macchi (Fondazione Bruno Kessler), Edel Sheridan (SINTEF), Elixabete Ayerbe (CIDETEC Energy Storage), Erwin Marckx (EUROBAT), Francesco Guaraldi (Flash Battery), Guillaume Muller (Solvay), Ivan Matejak (EERA), Javier Carrasco (CIC energiGUNE), Jesse Terry (BEPA Secretariat), Johanna Valio (Satakunta University of Applied Sciences / RoboAI R&D Center), Juan Enriquez (ANALISIS-DSC), Konrad Bendzuck (InnoEnergy), Luis de Prada (EUCAR), Maher Chebbo (Univers), Margherita Moreno (ENEA), Marco De Angelis (Department of Psychology, University of Bologna), Matteo Dotoli (Comau SpA), Mattia Felice Palermo (CIC energiGUNE), Mikko Pihlatie (VTT), Mohsen Shiea (Fondazione Bruno Kessler), Nga Thi Quynh Do (Technische Universität Braunschweig), Nicolas Vallin (Dassault Systemes), Panteleïmon Panagiotou (Bavarian Research Alliance), Peter Nemcek (CyberGRID), Philippe Jacques (EMIRI), Rudy Pastuzak (Dassault Systèmes), Simon Stier (Fraunhofer Institute for Silicate Research ISC), Spyridon Pantelis (EERA), Teresa Mata (INEGI – Institute of Science and Innovation in Mechanical and Industrial Engineering), Victor Gimeno Granda (Capital Energy), Ilka von Dalwigk (InnoEnergy), Jesse Terry (BEPA Secretariat), Lluís Trilla (IREC).

Acknowledgements: We would like to thank Spyridon Pantelis (EERA) for the overall coordination of the Task Forces, Alessandro Romanello (EIT InnoEnergy) as coordinator of Batteries Europe, and the BEPA Secretariat for their support in the operation of the Task Force. Special thanks to Fatima Ahmed, Adeola Adeoti, Lucia Sardone (CLERENS), and Maria Luisa Fernandez Vanoni (EERA) for editorial support. We would also like to acknowledge the inputs and considerations from the European Commission, the Batteries Europe Secretariat and Batteries Europe Advisory Board.

CONTENTS

EXECUTIVE SUMMARY			
1. IN	INTRODUCTION		
2. C	COMMON INFRASTRUCTURE, DATA SHAPES AND ONTOLOGIES		
3. A	ADVANCED MODELLING FOR ACCELERATED BATTERY DEVELOPMENT		
3.1	1 Automated discovery and design of battery materials		
3.2	3.2 Cell and battery design for emerging battery technologies		
3.3	3.3 Virtual battery testing		
3.4	3.4 Modelling tools for improved EOL, including sorting and recycling		
3.5	Battery value chain optimisation 15		
4. D	IGITAL TWINS		
4.1	Introduction		
4.2	Implementation of digital twins in the battery value chain		
4.	4.2.1 Battery cell manufacturing		
4.	4.2.2 Battery cell testing		
4.	4.2.3 Battery operation		
5. SC	5. SOX MONITORING		
5.1	SoH/SoC/SoE/SoP monitoring		
5.2	SoS monitoring		
6. C	ONCLUSION AND RECOMMENDATIONS		
6.1	Common infrastructure, data shapes and ontologies24		
6.2	Advanced modelling for accelerated battery development24		
6.3	Digital twins		
6.4	SoX monitoring		
6.5	General remarks on digitalisation28		
7. RI	EFERENCES		

ABBREVIATIONS AND ACRONYMS

Abbreviation	Definition
AI	Artificial Intelligence
BIG	Battery Interface Genome
BMS	Battery Management System
DPP	Digital Product Passport
EV	Electric Vehicles
EOL	End-Of-Life
FAIR	Findability, Accessibility, Interoperability, Reusability
THE	High-Throughput Experimentation
ICT	Information And Communication Technology
IoT	Internet Of Things
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LIB	Lithium-Ion Battery
MAP	Materials Acceleration Platform
ML	Machine Learning
PEFCR	Product Environmental Footprint Category Rules
SoX	State Of X
SoC	State Of Charge
SoE	State Of Energy
SoH	State Of Health
SoP	State Of Power
SoS	State Of Safety

EXECUTIVE SUMMARY

The Batteries Europe / BEPA Task Force on Digitalisation leveraged the activities of the Batteries Europe Working Groups to define the digitalisation agenda for batteries in Europe that was included in the Batteries Strategic Research Agenda.

Digital technologies are not a direct objective but an important enabler to achieve the development of innovative new services, the so called applications or use cases, leveraging technologies like digital twins, artificial intelligence (AI) and machine learning (ML), computer-aided design (CAD), data science, advanced modelling, 5G, blockchain or the battery passport that can deliver significant measurable benefits: saving costs, increasing revenues and setting up new business models, all contributing to achieve socio-economic benefits.

The current position paper presents some of these advanced technologies that could make a difference for the batteries industry. It illustrates these innovative technologies for the battery industry in the domains of engineering & design, manufacturing, maintenance, exploitation and recycling.

The native design of the battery hardware leveraging the digital technologies and continuous monitoring and control will enable the industry to optimise the state of multiple KPIs called SoX, like State-of-Health (SoH), State-of-Charge (SoC), State-of-Energy (SoE), State-of-Power (SoP), and the innovative concept of State-of-Safety (SoS) monitoring tools in battery management systems (BMS).

In conclusion, this report summarises recommendations for the central topics addressed within this position paper. These serve as guidelines for enabling advancement in the related technology domains across the whole value chain, targeting a wide range of stakeholders (s. section 5).



1. INTRODUCTION

Digital technologies have been used within energy systems for decades. The energy sector was one of the early adopters of large information and communication technology systems (ICT). Already in the 1970s, electric utilities used information and communication technology to aid the management of the transmission and distribution system. Many electricity markets around the world are monitored and controlled in real-time across large customer bases and geographic areas. Likewise, oil and gas companies have a long history of using digital technologies to aid exploration and production efforts. Similarly, a variety of industries have used process controls and automation to optimise energy use. Digital technologies have long been used across transportation modes to improve safety and increase energy efficiency. It is now a must have technology for electric cars to manage their batteries, and the same stands for stationary batteries that should integrate with the assets, such as buildings, renewables and electricity networks.

Blockchain, artificial intelligence (AI), machine learning (ML) and generative AI are digital technologies that are undergoing rapid development today and have the potential to bring disruptive changes to the energy landscape. Blockchain technology presents an exciting opportunity for decentralised energy environments to enable, validate, record, and settle energy transactions in real-time. Blockchain is a distributed digital ledger built on a decentralised transaction verification system; this framework could enable peer-to-peer transactions, where neighbours transact directly with each other, and trade energy generated from their rooftop solar panels and electric vehicles through the grid. These technologies play a major role in making batteries effective with an optimal lifecycle and payback cycles.

The EU Green Deal¹ and the digitalisation of the European economy, specifically the European energy system², will be important new priorities of the European Commission. Moreover, by 2050, renewables' share could reach as much as 87% in the electricity mix, with wind and solar energy playing a dominant role. Cheap renewables, flexible demand and battery storage will be digitally combined to shift the European power system away from fossil fuels and nuclear power to a cleaner society around variable renewables and emissions-free energy.

This shift in the energy transition will be enabled by smart digital technologies. Digital technologies will optimise the value that battery storage systems can bring to the energy markets, thereby enabling opportunities for new energy stakeholders, creating a new generation of jobs for the circular economy, and bring Europe to the forefront of leadership in the fight against climate change.

The development of digital technologies is required to improve the industrialisation of new batteries and shorten the time to market. The design of machine learning algorithms will accelerate the discovery of materials and the development of AI-orchestrated characterisation of battery materials and battery cells. Combining computer-aided engineering tools and experimental measurements will help to understand and predict the performance of batteries.

These technologies will continue to evolve more rapidly than the time required for the transformation within the mobility, storage and battery industries.

This position paper serves as an update to the last one published in 2021³ and focusses on recent technological aspects such as common infrastructure, data shapes and ontologies, digital twins, advanced modelling and state monitoring (SoX).

Therefore, it describes yet another step in the journey of an innovation-intense batteries industry.

2. COMMON INFRASTRUCTURE, DATA SHAPES AND ONTOLOGIES

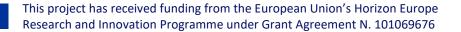
As a complex domain, battery research highly relies on agreed terminologies and standards. Beyond fundamental science (e.g., chemistry, physics, etc.), this was historically provided merely by verbal communications and lack of a global referenceable standards. Recent activities at national (e.g., German Battery Clusters) and European level (Battery2030+, LiPLANET, BIG-MAP) address this issue, for example by providing an interactive data space^{4,5}, a common knowledge base⁶ and battery related ontologies^{7,8}. However, to date, those initiatives have included only a small fraction of data produced by the research community. To generate a significant impact, they should be extended to a broad established framework and build a common battery knowledge graph consisting of linked and machine-readable self-descriptions of digital assets, providing domain knowledge, terminologies, tools, data shapes, etc.

To do so, it is important to acknowledge that ontologies, while being the technical foundation, will not serve as a direct interface to the general community. Instead, ontologies should be mapped onto pragmatic and real-world-reflecting data shapes, addressing both general (e. g. hierarchical description of a battery module down to materials) and specific needs within the domains (e. g. definition of a cycling procedure or electrochemical simulation input and output data). Accessibility to a growing collection of those linked data shapes can be achieved by auto-generating specific end user interface from those data shapes⁹.

By fulfilling not only data experts but also end users' needs, aligned ontologies, derived data shapes and generated interfaces are critical for upcoming data space initiatives, such as Catena-X¹⁰, which allow them to be effectively populated with content from a large community and enable data scientists, AI and simulation experts to provide shared digital services based on shared interoperable data.

Linking explicit machine-readable knowledge with experimental data in common battery data spaces will also serve as a basis for hybrid models to consider not only statistical and physical models, but also machine-readable expert knowledge. Likewise, machine-readable and consistent knowledge in form of process and material definitions will facilitate the application of sustainability evaluation tools, such as for Life Cycle Assessment (LCA), Digital Product Passports (DPP) and chains of custody. In consequence, implementing sophisticated semantic data and knowledge infrastructure will not only enable advanced internal process management and optimization, but also compliance with external regulations without additional costs.

LCA is a standardised methodology that has become the consensual tool of choice to assess the potential environmental impacts of products and processes throughout their life cycle. Although it is standardised by ISO 14040:2006 / ISO 14044:2006 and there are product environmental footprint category rules (PEFCR) for rechargeable batteries proposed by The Advanced Rechargeable & Lithium Batteries Association (RECHARGE), many assumptions are needed and different methods can be employed to quantify the environmental impacts. These facts increase the uncertainties of the results of environmental impact and hinder the comparison between different types of products. In this sense, there is a need for higher amounts and reliable primary data to support more robust LCA studies. Moreover, PEFCR should be developed and extended, not only for the battery as a product



on the system level, but also for its components and materials, e.g. data on the recycling of battery components like active materials and electrolytes. Additionally, considering a wide variety of output materials and different process technology readiness levels, a more consistent and ontology-based methodological approach should be developed for levelled comparison of the environmental impacts of different recycling processes. Furthermore, in the same way that environmental impacts are assessed using LCA methodology, economic and social impacts must also be assessed in life cycle thinking (LCT) perspectives, using the life cycle costing (LCC) and social life cycle assessment (s-LCA) methodologies^[1].

However, there are still significant questions regarding available data, in particular externalities costs and social data information.

For achieving interoperability of LCA standards (e.g. process flows and material exchange definitions) with material science and process engineering standards, the following actions are recommended:

- Use of the same ontology in the LCA documents for both chemical aspects at cell level and engineering/production process domain (e.g., carbon dioxide vs. CO₂).
- Implement the digital passport^[2] also for battery materials and parts within the supply chain, particularly in recycling materials. Develop a common ontology for battery passport (and digital twins) based on existing ontologies like the Battery Interface Ontology (BattINFO¹¹) and Battery Value Chain Ontology (BVCO¹²).
- Development of a Life Cycle Inventory (LCI) database, or LCI datasets, specifically intended to be used in the development of LCA studies or in the creation of DPPs. To ensure the representativeness of the LCA and sustainability studies carried out based on this data, specific data transfer and storage formats must be defined, considering the information that must be provided and how it must be obtained. Moreover, specific measures should be taken to protect sensitive information, for example intellectual property or business information, using protocols such as blockchain or others created specifically for battery systems. In addition, data formats should facilitate the assessment of environmental impacts, based on existing or future product category rules (PCR) or methodologies created for DPPs. Efforts should be made to ensure that all data is open source and can be incorporated into existing or future open source LCI databases, of general nature such as the environmental footprint database¹³ or tailor-made for battery systems. Future LCI databases should be updated periodically and allow for the submission of new data, considering the applicable data formats. This aspect is relevant for small and medium-sized companies, for whom carrying an LCA study and/or developing DPPs can represent an excessive expenditure of resources.



 ^[1] more information on LCA and s-LCA provided in position paper of Task Force Sustainability: <u>https://batterieseurope.eu/workstream-bodies/cross-cutting-task-forces/</u>
^[2] see also position paper of Task Force Sustainability: <u>https://batterieseurope.eu/workstream-bodies/cross-cutting-task-forces/</u>

3. ADVANCED MODELLING FOR ACCELERATED BATTERY DEVELOPMENT

The battery sector is growing very rapidly and to remain competitive, companies need to accelerate their development efforts and reduce the time-to-market. Digital technologies can be a key enabler for the industry, also thanks to the ever-growing availability of computational resources and the continuous advances in modelling, coming from the scientific community. Advanced modelling and digital technologies can provide valuable support in different phases of the battery development process, but also during the deployment phase, targeting the optimisation of the entire battery value chain. Starting from the material level, automated discovery and design of battery materials can be a key enabler for the development of innovative energy storage technologies and for the continuous improvement of the currently consolidated chemistries. Advanced multiphysics-multiscale models are also crucial to support the development and design of battery cells and systems for emerging battery technologies. Battery development currently still requires complex, time-consuming and expensive testing. Digital tools can be used to minimise the need of physical testing, integrating virtual testing in the standard development process to evaluate battery performance, lifespan, reliability, and safety. Advanced modelling can also be used to design and optimise new recycling processes and additionally to evaluate how these processes can deal with the upcoming battery chemistries. Finally, digital tools can support the optimisation of the entire battery value chain and logistics, linking all steps, from raw material extraction to end-of-life (EOL), to ensure the lowest environmental impact and reduce total costs.

Adopting an open-source software approach to the development of these digital solutions will ensure scalability, flexibility and, above all, adaptability to different battery technologies, greatly benefitting the European Battery Industry.

3.1 Automated discovery and design of battery materials

The integration of automated discovery in battery development via high-throughput experimentation and advanced modelling has emerged as a key enabler in developing novel energy storage technologies. These methods allow for a more expedited development process, while at the same time contributing to the reduction of R&D costs and in obtaining superior battery performance^{14,15}. This section aims to explore how these methodologies have been developed within the framework of the current EU initiatives and sets the expectations for the upcoming years, aligning with the vision and strategic objectives outlined in the Battery 2030+ roadmap¹⁶.

High-throughput experimentation (HTE) allows for the simultaneous screening, synthesis and characterisation of large arrays of different material classes, which can lead to the identification of lead candidates for given systems and targeted applications^{17,18}.*Computational modelling*, encompassing electronic structure calculations, atomistic and molecular simulations, continuum modelling, and data-driven and predictive modelling, enables a comprehensive exploration of electrochemical, mechanical, thermal and structural properties of battery materials^{19,20,21}. Over the recent years this approach has accelerated the ability to explore and optimise battery design,



expediting the research process and opening new pathways for innovation in battery technologies¹². Furthermore, machine learning and artificial intelligence are emerging as enablers to create faster and more accurate models with improved prediction accuracy, better generalisation to new conditions and the ability to incorporate complex battery behaviours.

The BIG-MAP project²², under the Battery 2030+ initiative roadmap²³, currently represents the largest effort in developing an automated ecosystem for chemistry and technology-neutral battery material discovery. Within BIG-MAP, the materials acceleration platform (MAP) focuses on the autonomous acquisition, handling and analysis of comprehensive data sets, encompassing the full spectrum of the battery development cycle. In conjunction with MAP, the battery interface genome (BIG) initiative focuses on understanding critical battery processes happening at the interfaces, such as charge transfer reactions, dendrite formation, solid electrolyte interphase formation, and cathode–electrolyte interface development. Building upon the foundational work of MAP, BIG seeks to establish a comprehensive understanding of these interface-related processes, which are vital for the functioning of all batteries.

Additional EU initiatives with a narrower focus include the SONAR and OPERA²⁴ projects. The former aims to establish a framework for evaluating electroactive materials suitable for aqueous and non-aqueous redox flow batteries. This will involve a multiscale modelling approach that enhances and connects simulation methods across different scales through a blend of physics and data-driven modelling. The OPERA project aims to revolutionise solid-state batteries by developing new operando techniques and multiscale modelling strategies. These efforts are focused on understanding and optimising the interfaces within these batteries, with the aim of achieving zero-excess energy storage.

Beyond the EU initiatives, there is a significant global effort directed towards the development of computational techniques to understand and develop new battery technologies.

The advancement of HTE in battery research is increasingly characterised by an interplay between automated processes and computational models. Central to this is the accelerated experimental design of anodes, cathodes and solid electrolytes for Lithium and beyond Lithium batteries. This approach is crucial for assessing extensive candidate lists derived from combinatorial studies and for enhancing the robustness of machine learning models²⁵. Complementary to this trajectory is the advent of MAPs, which combine AI, robotics and computing. These platforms expedite the experimentation process, although they are still navigating the complexities of achieving full autonomy²⁶.

The effective utilisation of the data generated from these technologies is a critical aspect, necessitating the integration of AI/ML algorithms. This integration is essential for enhancing decision-making processes in the development of battery materials, streamlining the journey from theoretical models to practical applications¹⁵. The role of AI/ML in this domain is recognised for its transformative potential. It is not just about accelerating research but also about making these tools accessible and applicable across various research contexts²⁷.

The global response to environmental and material challenges underscores the urgency of accelerated discovery in battery research. MAPs are at the forefront of this endeavour, advocating for a collaborative approach across industries and borders. Such collaboration is vital to achieve sustainable solutions, aligning technological advancements with the global imperative for environmental sustainability and resource efficiency²⁸.



3.2 Cell and battery design for emerging battery technologies

The battery sector is evolving very rapidly due to the large demand for batteries for both mobility and stationary applications. In this context, upcoming and emerging battery technologies will play an important role, enabling to diversify the supply of the needed materials and achieving the targeted costs and performances needed for each application sector. The availability of validated models and software tools is crucial to accelerate the technology development and reduce the time-to-market for these new battery technologies.

Models and software for lithium-ion battery (LIB) design and optimisation from cell to battery pack are currently commonly used and readily available with both commercial and open-source options, e.g., COMSOL²⁹, Ansys Fluent³⁰, PyBaMM³¹, BattMo³², cideMOD³³. However, validated models and tools for upcoming and emerging battery technologies such as redox flow batteries (excluding vanadium redox flow battery), solid-state batteries, metal-air and metal-sulphur are still missing. For each battery technology, the required activities concern:

- The development of multiphysics mathematical models of increasing complexity to reproduce the physical phenomena affecting the cell performances;
- The implementation of the models in state-of-the-art computational tools;
- Model validation based on accurate and complete experimental datasets.

Each of these activities is crucial to ensure that the European battery industry has the needed tools to build better and lower cost storage technologies.

Battery models need to take into account several physical phenomena (chemical, electrical, thermal, mechanical) and their interactions which happen at different scales, from electrode to the system level. Each scale requires different modelling approaches that can be integrated into a multiscale modelling tool optimising this way the overall battery design. The core component of such a tool would be a continuum-scale multiphysics model for battery cell that can also be used to develop battery packs/stacks (either directly or indirectly through model order reduction).

The integration of such models in open source tools would greatly benefit the whole battery industry and community, also removing the cost barriers that can limit small companies in getting access to validated tools from commercial providers. The use of state-of-art open source computational software, such as those developed in Python, OpenFOAM, FEniCS and MATLAB, will ensure scalability, flexibility and most of all the adaptability to different battery technologies. The long-term target would be an integrated multiscale tool that could address the different industry needs. Streamlining the development efforts of the European scientific community into a single direction of an open multitechnology battery toolkit serving our European battery industry could bring important benefits in the long run.

3.3 Virtual battery testing

The current approach to battery development primarily relies on trial-and-error methods, which are time-consuming and expensive, and do not always yield optimal product designs. Existing methods and tools often incur high costs due to long test periods, the need for a large number of test samples,



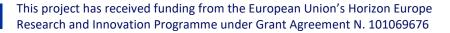
and the utilisation of expensive testing infrastructure. However, there is a significant potential for enhancement by leveraging digital methods and tools to minimise reliance on traditional trial-anderror processes to evaluate battery performance, lifespan, reliability, and safety. The digitalisation of battery testing will result in faster battery development, shorter time-to-market, enhanced evaluation of performance, lifespan, reliability, and safety and more accurate estimation of battery lifespan through improved modelling of battery aging and the use of digital twins. These advancements in battery testing will lead to substantial cost savings, particularly during the development phase. Recently, several initiatives have been funded by the EU to fill the existing gap, e.g., AccCellBaT³⁴, THOR³⁵, FASTEST³⁶ and DigiBatt³⁷. However, several challenges still need to be addressed.

One of the main challenges concerns the development of virtual methods to reduce the complexity, costs and time related to testing from cell to system level. Integration of models (both physics-based and data-driven) with real data coming from physical testing at smaller scale or sub-component level will reinforce the prediction capabilities of these methods. Research is also needed on the standardisation of battery system testing & validation approaches focusing on the fusion of physical and virtual test methodologies. These approaches, combined with the development of simplified testing strategies, will make it possible to reduce the number of physical tests required and their complexity, while improving the safety and reliability of batteries. Finally, it is crucial to understand the impact of different operating loads, failure modes, ageing and misuse on battery reliability and safety of batteries and to highlight the dependencies between them in order to design the most adequate testing methods and parameters.

3.4 Modelling tools for improved EOL, including sorting and recycling

The transition towards a circular economy requires sustainable waste management to reduce its adverse impacts on the environment and human society. Such a management should close the product value chain to reduce the use of resources and raw materials, ensuring current and future access to these resources. This is strategically important for a secure and sustainable supply of critical raw materials to increase resilience and security of a society. In the context of batteries, the EU has already implemented appropriate measures (e.g., EU battery Regulation), to ensure the development of a sustainable circular value chain for batteries in Europe. In this regard, recycling plays a key role in closing the value chain of different battery technologies. In fact, the EU Battery Regulation establishes strict measures on the recycling efficiency of end-of-life batteries and the amount of recycled material to be used in manufacturing of new batteries. Therefore, great attention should be paid to developing recycling processes that comply with battery regulations, especially in view of the lack of established sustainable and economic recycling routes for current and next generation lithium-ion batteries, batteries based on new chemistries and other battery technologies such as redox flow batteries. In this regard, the use of models to bridge the gap in battery recycling is crucial to keep up with the increasing pace of technological change fostered by the influence of digitalisation in various fields.

An interesting topic is the development of reliable physics-based models for chemical processes that have potential use in the recycling of batteries. These models can be used to assess the viability of the processes developed for new battery chemistries and technologies. In addition, they can facilitate the scale-up, optimization and control of chemical processes to achieve higher recycling efficiency, lower energy consumption and reduced CO₂ emissions. For instance, the hydrometallurgical recycling route





for end-of-life Li-ion batteries relies on chemical steps such as leaching, liquid-liquid extraction and precipitation. And reliable models can facilitate the development or adaptation of these steps as new chemistries are introduced into the market. Focusing on the diversity of chemistries, promising modelling frameworks can be beneficial to evaluate the flexibility of a particular process to handle changes in the composition of feeds received by recycling plants. In addition to physics-based models, data-driven or hybrid approaches are needed to estimate the performance of those recycling steps for which a physical description is not yet available.

Another topic of interest is the direct recycling of battery active materials, particularly for Li-ion batteries. Models, either physics-based or data-driven, can serve to predict the nature of degradation of active materials by examining the battery's life history, possibly available through the battery passport, which is essential for successful direct reconditioning of active materials.

Lastly, it is important to note that modelling tools for steps of recycling processes can be integrated into digital twins of recycling plants for the purpose of process control and optimized operation.

3.5 Battery value chain optimisation

In advancing our research approach within the battery research and industry, one of the main priorities is to bridge the gap between digital tools and the entire value chain, from raw material extraction to manufacturing, product utilization and eventual recycling. Traditionally, research has been compartmentalized into specific elements within the battery value chain, often overlooking the need for a holistic perspective. To achieve a comprehensive understanding, it is imperative to establish connections between these elements and integrate them into a larger framework. This integration necessitates interoperable data structures that facilitate connectivity between neighbouring domains and contribute to optimizing the entire value chain for sustainability (s. section 2).

Leveraging forward and reverse computer aided engineering techniques is crucial in this endeavour, allowing us to refine designs and processes iteratively. The application of *digital product life cycle management* serves as an aggregating concept, ensuring a seamless flow of information and insights throughout the entire life cycle.



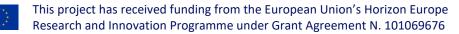
4. DIGITAL TWINS

4.1 Introduction

The concept of the *digital twin* has gained significant attention since it was first mentioned in a NASA publication in 2010^{38,39}. Digital twin is understood in this chapter as a virtual representation or digital counterpart of a physical object, process, system or entity that incorporates real-time data and simulation capabilities, enabling it to accurately reflect the behaviour and changes of its physical counterpart over time.

There are numerous examples that illustrate the versatility and wide-ranging applications of digital twins in various industries, demonstrating how they contribute to improving efficiency, decision making and overall performance. In this context, core elements describing a digital twin are the physical world, the virtual world, and the flow of data between the physical asset and its virtual representation⁴⁰. The quest of developing battery digital twins involves several technical advancements across various domains. Here are all key areas that should be considered in order to succeed in building robust and reliable DTs in the battery sector:

- **High-fidelity battery models**: Develop advanced battery models that accurately represent the real assets, incorporating detailed physics to simulate battery manufacturing and performance under different operating conditions.
- **Real-time monitoring and diagnostics**: Implement robust real-time monitoring systems to collect data on key battery parameters. Additionally, this implies the integration of sophisticated diagnostic algorithms capable of detecting early signs of degradation, faults, or abnormal behaviour.
- Sensors and instrumentation: Explore and implement novel sensor technologies to enhance the granularity of data collection, capable of monitoring internal conditions within the whole battery value chain.
- **Data integration**: Establish frameworks for seamless integration of data from various sources, including sensors, historical performance data, and external environmental factors. This should also include the implementation of data fusion techniques to create a comprehensive and accurate representation of real assets.
- Machine learning algorithms: Utilise machine learning algorithms to analyse vast amounts of data and identify patterns. Then train models to predict future battery performance based on historical data and real-time input.
- **Cyber-physical systems integration**: Integrate the digital twin with the physical assets through cyber-physical systems, enabling bidirectional communication and control. This might imply the establishment of secure communication protocols to ensure the reliability and integrity of data exchanged between the physical battery and its digital twin.



- Adaptive control strategies: Develop adaptive control strategies that leverage insights from the battery digital twin to optimise charging and discharging protocols in real-time. This would involve the implementation of algorithms that dynamically adjust operating parameters to maximise performance while minimising degradation.
- User interface and visualisation tools: Design user-friendly interfaces and visualisation tools to enable users to interpret and interact with the digital twin. Such interfaces should then be able to provide actionable insights and recommendations for maintenance or operational adjustments based on the digital twin's analysis.
- **Continuous learning and improvement**: Establish mechanisms for continuous learning and improvement, allowing the battery digital twin to adapt and evolve over time as new data and insights become available.
- Integration of the digital twin in the company management system: The integration of the digital twin with other tools, as for example enterprise resource planning software or product life cycle management tools. This will allow a more effective practical utilisation of digital twin in practice, and even to incorporate economic and/or environmental parameters in it. Furthermore, this approach will enable leveraging the digital twin for supporting process improvement and optimisation, while also facilitating the comprehensive integration of batteries lifecycle into those processes

Here are additional considerations related to security, standards, and communication that are important to pay attention to while developing digital twins:

- **Digital twin validation**: A key aspect when developing, implementing, and using in practice a digital twin is the question of how well it represents reality. Hence, special attention should be given to its validation, that should be based as much as possible on real life of the process operations, or from the stakeholders of the battery value chain. Questions of data quality and/or uncertainty should be addressed here when performing the validation.
- **Digital twin updating**: As technology, regulations, strategies, and other relevant aspects directly related to the battery sector keep evolving, updates of the implemented digital twin are required from time to time. This can be an activity with a defined periodicity or done when it is required. In this updating process, data and/or information from the various stakeholders involved in the battery value chain should be used to ensure that the new iteration of the digital twin improves when compared do the previous one.
- **Communication protocols** that facilitate communication between the physical object, sensors, and the digital twin. Common protocols include MQTT (Message Queuing Telemetry Transport), CoAP (Constrained Application Protocol), and HTTP (Hypertext Transfer Protocol).
- **Cybersecurity protocols** and measures to protect the digital twin and the data it handles from unauthorised access, breaches, and cyber threats. The new protocols may be based on already existing data exchange and traceability, as for example blockchain, or specifically designed for battery systems.





• Adherence to **industry standards and protocols** to ensure interoperability, compatibility, and consistent data exchange between different digital twin implementations.

The integration of these elements and considerations will ensure the creation of a robust, accurate, reliable and effective Digital Twin system, capable of providing valuable insights, optimising processes, and facilitating better decision-making. Additionally, addressing communication, security, and industry standards will enhance the reliability and trustworthiness of the digital twin environment.

4.2 Implementation of digital twins in the battery value chain

The digital twin concept is recognised as a pivotal element in the digitalisation era of the entire battery value chain. Thus, from the initial conception phase through the manufacturing process, where raw materials are transformed into cells meeting specified requirements, to the critical testing phase encompassing crucial steps such as formation and aging studies, the digital twin emerges as a vital method for accelerating the development phase.

4.2.1 Battery cell manufacturing

The scope of digital twins in battery cell production is very broad and can range from a digital twin of a building to a digital twin of a machine or asset, to a digital twin of a product (i.e. battery cell)⁴¹. *Digital twins for buildings* usually describe the building information model (BIM) and aggregate contents of environmental effects and dependencies such as energy consumption, logistic simulations and building automation for monitoring and control. This will enable building managers to make data-driven decisions and adjustments before the actual operation. On the other hand, *digital twins for machines* provide a dynamic and responsive representation of a manufacturing equipment, offering benefits such as adaptive processes, predictive maintenance, and overall operational optimisation. Furthermore, a *digital twin of a product s*erves as a virtual representation that captures and integrates information throughout the entire production process⁴².

The successful integration of digitalisation approaches in an automated production line holds the promise of significantly reducing the overall costs of battery cell production. By leveraging digital technologies such as internet of things (IoT) and AI/ML, manufacturers can streamline processes, optimise resource utilisation, and minimise waste, leading to increased efficiency and cost savings. Automation allows for precise control and monitoring of production parameters, resulting in higher quality output and fewer defects. Additionally, digitalisation enables real-time data analysis and predictive maintenance, helping to prevent costly downtime and equipment failures. Overall, the integration of digitalisation in battery cell production represents a key strategy for improving competitiveness and sustainability in the industry.

4.2.2 Battery cell testing



The concept of a digital twins in cell testing follows a similar philosophy to other digital twin applications, such as digital twin manufacturing and state-of-health (SoH) estimation control. The primary focus is on leveraging virtual representations to accelerate and enhance the understanding of the performance of cells being tested in the laboratory. In this context, digital twins in cell testing will aim to accelerate the testing processes by providing a virtual environment where simulations and analyses will be performed, reducing the time required for physical testing and allowing for a more rapid iteration of experiments. Additionally, integrating real-time data from physical tests into the digital twin will enhance its accuracy and reliability and will give the opportunity to researchers to compare virtual predictions with actual test results. As a result, this will enable the improvement of the digital twin model over time.

In essence, the digital twin concept in cell testing is a powerful tool for researchers seeking to advance their understanding of battery cell behaviour. It aligns with the broader trend of leveraging digital twins across various industries to enhance efficiency, optimise processes, and drive innovation.

4.2.3 Battery operation

The effective and efficient management of lithium-ion batteries is crucial for low-carbon applications, such as electric vehicles and grid-scale energy storage. The lifetime of these batteries is intricately tied to various factors, including materials, system design, and operating conditions. The complexity of factors affecting battery performance has made real-world control of battery systems challenging and recent advancements in understanding battery degradation, modelling tools, and diagnostics present an opportunity to overcome these challenges. In this context, there is a prospect to integrate knowledge about battery degradation, modelling tools, and diagnostics with emerging machine learning techniques. This integration aspires to the birth of the concept known as the *battery digital twin*, which involves a close interaction between the physical battery and its digital representation. The envisioned outcome is a battery digital twin that facilitates smarter control, ultimately allowing for a more intelligent and interconnected approach contributing to a potentially extended battery lifespan^{43,44,45,46}.

The successful integration of these technical developments will pave the way for a sophisticated battery digital twin, revolutionising the management and optimisation of batteries in diverse applications. Additionally, the deployment of sophisticated battery digital twin frameworks might enable strategies for the second use of batteries. In particular, leveraging accurate battery models, continuous monitoring systems, and advanced sensors, such frameworks could assess the remaining useful life of batteries post their primary application. For example, by integrating data from historical performance and employing machine learning algorithms, these models could predict the performance of batteries in potential second-life scenarios. Moreover, the cyber-physical integration ensures real-time insights, enabling decision-makers to evaluate a battery's health and suitability for repurposing. This, of course, should imply security measures, including robust protocols for data handling, addressing privacy concerns associated with the battery's first-life information. Overall, by identifying batteries suitable for a second life, the digital twin concept helps in reducing the generation of electronic waste.



5. SOX MONITORING

In the rapidly evolving landscape of energy storage, the efficient management of Lithium-Ion batteries (LIB), in particular for electric vehicles (EV), has emerged as a critical concern. It is paramount to maximise battery pack performance in real time operation, ensuring safety, optimising energy efficiency, while at the same time obtaining accurate assessment of the battery's health and operating conditions. In this regard there is a significant need for implementing State-of-Health (SoH), State-of-Charge (SoC), State-of-Energy (SoE), State-of-Power (SoP), and the innovative concept of State-of-Safety (SoS) monitoring tools. These terms are collectively referred to as state of X (SoX), in battery management systems (BMS) for the batteries of the future (see *Figure 1*).

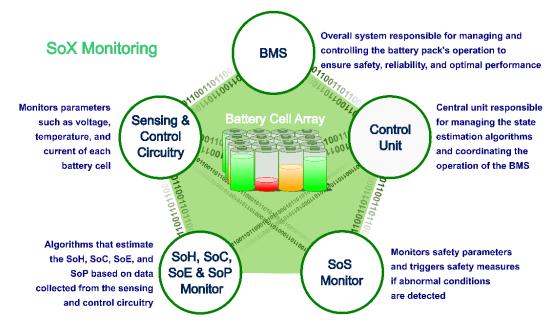


Figure 1: Integrating digital technology to create SoX monitoring systems for enhanced battery performance and safety.

5.1 SoH/SoC/SoE/SoP monitoring

SoH, the remaining capacity relative to the original capacity, stands as a key indicator in understanding the degradation performance of LIBs. Accurate SoH estimation is essential for prolonging battery lifespan and preventing unexpected failures. Traditional approaches, such as *Coulomb counting* ^[3] and model-based estimation, have paved the way for reliable SoH assessments but often require a full charge/discharge cycle, a process that can be time-consuming and lengthens the diagnostics phase. This is because these methods rely on capturing comprehensive data throughout the entire charging and discharging process to accurately assess the battery's health status. The recent introduction of digital twin frameworks offers a paradigm shift by enabling real-time SoH estimation without the need for complete discharge cycles. This capability not only enhances the accuracy of SoH assessment but

^[3] calculating the remaining capacity by accumulating the charge transferred in or out of the battery



also allows for proactive measures to be taken during ongoing cycles, minimising the risk of unexpected degradation.

Both SoC, representing the current level of charge stored in the battery, and SoE, describing the residual energy of the battery cell under specific operating conditions, play a crucial role in determining the energy availability of a battery. SoP is analogous to SoC but pertains to power rather than charge^[4], considering factors such as the current charge level, internal resistance, and the ability of the BMS to regulate power output.

Effective SoC and SoE monitoring ensures optimal utilisation of the battery's capacity and energy, respectively and are integral for the reliable operation of devices. SoP is important in applications where the instantaneous power demand fluctuates rapidly, such as EVs or grid stabilisation systems. Maintaining an adequate SoP ensures that the system can respond quickly to changes in power demand without experiencing voltage drops or power delivery limitations. In this context, industrial internet of things IIoT-based digital twin frameworks, employing advanced data-driven approaches to estimate SoC/SoE/SoP in real-time, can be expected to become key enablers for technological advancement. This approach not only overcomes the challenges associated with complex battery dynamics and varying operating conditions, but could also contribute, for example, to accurate determination of EV range. The integration of this technology can revolutionise the efficiency of EVs and other applications reliant on LIBs.

From a BMS perspective, accurately assessing SoH/SoC/SoE/SoP of LIB cells typically implies combining the monitoring of voltage and current signals. Practical implementations in BMS essentially fall into three primary categories^{47,48}:

- **Coulomb counting methods**: These methods involve a simplified analytical representation of the battery, using current integration to compute SoC and SOP. SoH is updated by referencing manufacturer datasheets.
- Model-based estimation methods: In this approach, battery cell models are employed to deduce SoC/SoH. One widely-used model type is the one based on electrochemical models due to their strong abilities to capture both kinetic and charge transfers inside a battery, further resulting in a highly accurate SoC indication. Another model type is the equivalent circuit model that utilises the electrical circuit components to emulate battery dynamics. Online estimators or adaptive filters correct measurement errors and deviations from the estimation. This method enhances accuracy by leveraging predictive models.
- **Data-driven methods**: Using an input-output approach (black-box models), this method employs estimators based on fuzzy controllers, neural networks, and support vector machines. These data-driven techniques do not rely on detailed knowledge of the battery's internal mechanisms and can adapt to various scenarios.

These methodologies offer diverse approaches to assess battery cell states, each with its strengths and applications. Coulomb counting provides simplicity and reliance on manufacturer data, model-based estimation enhances accuracy through predictive models, and data-driven methods offer flexibility by

^[4] i.e. typically refers to the available power output capability of a battery at a given moment



utilising black-box models for estimation. The choice of the most suitable method depends on specific application requirements and the level of detail and adaptability needed in the assessment process.

5.2 SoS monitoring

Introducing the concept of SoS can further elevate the monitoring capabilities of BMS. SoS encapsulates the overall safety status of the battery, considering factors such as thermal stability, internal resistance, and the potential for catastrophic events. However, tackling real-time monitoring of SoS requires a holistic approach to battery data management. What sets SoS apart from other states is its impartial nature. Unlike SoH/SoC/SoE/SoP, which consider tailored estimators for distinct applications, SoS focuses solely on the possibility of a dangerous reaction at any given moment, quantifying the risk even when the storage system is inactive. This distinguishing feature renders SoS applicable to various energy storage systems beyond batteries, encompassing fuel cells and supercapacitors, given the identification of appropriate safety limits.

Integrating SoS into BMS aligns seamlessly with existing charging and energy management systems prevalent in EV and charging stations. The ability to calculate SoS online, akin to the online estimation of SoC, empowers the BMS to make real-time decisions aimed at reducing the likelihood of abuse and potential hazards. A notable example involves a car manufacturer responding to a fire incident post-charging by introducing a software update to mitigate unsafe charging conditions, underscoring the adaptability and proactive nature of SoS implementation. In hypothetical scenarios, SoS could prove invaluable in post-event calculations, such as after a mild EV crash. Leveraging information from sensors pre- or post-crash, the BMS could calculate SoS, providing critical warnings to passengers and first responders about imminent hazards. This potential application showcases the real-world impact of SoS in enhancing safety protocols and response mechanisms.

From a practical viewpoint, a promising avenue for estimating SoS in BMS is the digitalisation of impedance measurements. Several methods can be envisioned:

- Real-time monitoring with online impedance analysis: Implement real-time monitoring of impedance over a range of frequencies using digitalised measurements during the battery's operation. This continuous analysis can allow for the immediate detection of deviations from normal impedance levels, offering insights into aging mechanisms and signalling potential safety risks.
- Machine learning algorithms for pattern recognition: Integrate ML algorithms that can analyse patterns within the digitalised impedance measurements. Train the ML model to recognise abnormal impedance behaviour associated with hazardous conditions, enabling the BMS to predict and mitigate potential safety issues.
- **Correlation with environmental factors**: Correlate digitalised impedance measurements with environmental factors such as temperature and humidity. Changes in these variables can impact battery safety, and by integrating them into the analysis, the BMS can enhance its ability to estimate SoS accurately.



- Digital twin framework for predictive analysis: Develop a digital twin framework that replicates the battery's behaviour using digitalised impedance measurements and communicates with the physical battery. This virtual representation can undergo predictive analysis to simulate various operating conditions, helping the BMS anticipate safety concerns before they manifest in the physical battery (s. section Error! Reference source not found.).
- Integration of multi-sensor data: Combine digitalised impedance measurements with data from other sensors within the battery system. Integrating information on voltage, current and temperature alongside impedance can provide a holistic view, enhancing the BMS's ability to estimate SoS accurately.
- Advanced signal processing techniques: Apply advanced signal processing techniques to digitalised impedance data. Techniques such as wavelet analysis or Fourier transforms can extract valuable information from impedance measurements like distribution of relaxation times (DRT), aiding in the identification of potential safety risks and help estimating different aging routes that might be used to change battery management strategies to increase remaining useful life (RUL)
- **Continuous calibration and validation**: Implement a continuous calibration and validation process for the algorithms used in digitalised impedance analysis. This ensures that the SoS estimation remains accurate over time, accounting for variations in battery behaviour and characteristics.

By integrating these methods, a BMS can harness the power of digitalised impedance measurements to estimate SoS effectively, offering a proactive and data-driven approach to battery safety management. Moreover, the accuracy and reliability of SoS assessment methods can be further bolstered by refining its subfunctions and adjusting existing parameters. While safety limits can be initially chosen through empirical methods, the wealth of global battery safety tests provides an opportunity to incorporate more statistical data. Additionally, delving into the probabilities of failure for individual components, such as electrodes, separators, and electrolytes, presents avenues for enhancing the predictive capabilities of SoS. Crucially, the interlinked nature of SoS subfunctions, akin to a chain, emphasises that the overall safety is determined by the weakest or most unsafe link. This inherent connectivity underscores the need for comprehensive research to fortify each subfunction, ensuring that safety metrics decrease rapidly as necessary.

Overall, SoS heralds a new era in battery safety management, offering a quantifiable measure of potential hazards independent of usage scenarios. Its digitalisation and integration into BMS promise a proactive approach to safety, adaptable decision-making, and enhanced response capabilities. The ongoing refinement of SoS through research on subfunctions and component probabilities underscores its potential to redefine safety standards across diverse energy storage systems. As the energy landscape continues to evolve, SoS stands as a beacon, illuminating the path toward safer, more resilient energy storage technologies.

6. CONCLUSION AND RECOMMENDATIONS

In conclusion, the following recommendations summarise the most important topics addressed within this position paper and can be used as a guideline for enabling advancement in the related technology domains

6.1 Common infrastructure, data shapes and ontologies

Common data structures, aligned ontologies, derived data shapes, and generated interfaces are crucial for data space initiatives such as Catena-X⁴⁹. These structures and frameworks facilitate the population of data spaces with content from a diverse community, enabling data scientists, AI/ML experts, and simulation experts to offer shared digital services based on interoperable data. By

• Common data structures, ontologies, data shapes, and interfaces are crucial for Catena-X and other data space initiatives, enabling shared digital services.

Batteries + Europe

- Implementing a digital passport system for batteries should be based on Catena-X and domain ontology like BattINFO and BVCO.
- Linking machine-readable knowledge with experimental data in battery data spaces allows for hybrid models that combine statistical, physical, and expert knowledge.
- Consistent ontologies in both sustainability and materials, engineering and production research will enable sustainability by design with early feedback loops

linking machine-readable knowledge with experimental data in battery data spaces, hybrid models can be created that incorporate statistical and physical models alongside expert knowledge. The use of a consistent ontology in life cycle assessment (LCA) documents for both chemical aspects at the cell level and the engineering/production process domain is recommended. Additionally, it is suggested to implement a digital passport system for battery materials and parts within the supply chain, especially for recycling materials. This should involve the development of a common ontology for battery passport and digital twins, building upon existing ontologies like BattINFO⁵⁰ and BVCO⁵¹.

6.2 Advanced modelling for accelerated battery development

Advanced modelling and digital technologies are becoming a key asset for accelerating the battery development process. The advancement of battery materials through automated discovery hinges on a holistic approach, integrating computational predictions with experimental data to deepen our understanding of battery behaviour and validate models effectively. This entails aligning goals across academic and industrial sectors to ensure cohesive progress. Open science and collaboration are key drivers, advocating for transparency and efficient academia-industry partnerships. A balanced research approach, embracing both technology-neutral foundational research and specialised investigations, fosters knowledge exchange and synergy between diverse research teams. Establishing a centralised repository of automated methodologies, workflows, and protocols, with clear and extensive

will documentation, maximise resource utilisation and accessibility. Additionally, developing interoperable data infrastructures and ontologised archives will facilitate access to highquality FAIR data (findability, accessibility,

interoperability, reusability), integrating computational platforms with experimental data for high-throughput calculations.

In addressing emerging battery technologies and virtual battery testing, developing validated models and software tools for redox flow batteries, solid-state batteries, metal-air, and

- Establish a centralised repository of automated methodologies, workflows, and protocols with clear and extensive documentation.
- Develop interoperable data infrastructures and ontologised archives.
- Develop validated models and software tools for, e.g., redox flow batteries, solid-state batteries, metal-air, and metal-sulphur systems, among others.
- Prioritise multiphysics mathematical models integrated into open source computational platforms.
- Integrate physics-based and data-driven models with real data.
- Implement standardised battery system testing and validation approaches, focusing on the fusion of physical and virtual methodologies.
- Develop reliable **physics-based models for chemical processes** involved in recycling.
- Integrate modelling tools into digital twins of recycling plants for process control and optimization.
- Bridge digital tools across all stages, from raw material extraction to recycling, to optimise the battery value chain.

metal-sulphur systems, among other, is paramount. This includes prioritising multiphysics mathematical models integrated into open source computational platforms to ensure scalability and flexibility across battery technologies. Integrating physics-based and data-driven models with real data will enhance prediction capabilities and reduce complexity, costs, and time associated with physical testing. Standardizing battery system testing and validation approaches, focusing on the fusion of physical and virtual methodologies, will improve safety and reliability. For battery end-of-life (EOL) and recycling, developing reliable physics-based models for chemical processes involved in recycling will optimise efficiency, energy consumption, and CO₂ emissions. Integrating modelling tools into digital twins of recycling plants for process control and optimisation will enhance overall efficiency and performance.

AI/ML plays a crucial role, demanding the development of models that harmonise predictive power with physical constraints, trained on comprehensive datasets covering synthesis to testing phases. Moreover, exploring novel AI/ML architectures such as transformer models can enhance molecular modelling and property predictions. Multiscale modelling bridges simulations across various scales, leveraging machine learning for parameterisation and model scaling. Advancements in automated characterisation and synthesis are essential, requiring the refinement of high-throughput methods and the establishment of efficient infrastructures for sample transfer and testing.

Finally, optimising the battery value chain necessitates bridging digital tools across all stages, from raw material extraction to recycling. This comprehensive approach ensures the integration of digital methods with traditional processes, fostering sustainability and efficiency across the entire battery value chain.



In summary, the integrated approach outlined emphasises coordinated efforts across disciplines, transparent knowledge dissemination, and the strategic utilization of AI and multiscale modelling to drive innovation in battery material discovery.

6.3 Digital twins

The versatility and potential applications of digital twins across different actors have contributed to the absence of a single, comprehensive definition of the digital twin. While there are general understandings of what digital twins entail, their specific implementation and scope can vary significantly depending on the context

- A **sophisticated battery digital twin** will be indispensable across the entire battery value chain.
- These transformative digital twins will revolutionise battery management and optimisation across diverse applications, spanning from initial conception and manufacturing to testing stages and final usage.
- Overcoming challenges such as the lack of standards, models, interoperability issues, and efficiently integrating real-time data into a centralised data warehouse, digital twins will serve as a cornerstone for accelerating battery development, reducing cost, and promoting environmental sustainability.

and target. This flexibility is both a strength and a challenge, as it allows organisations to tailor digital twins to meet their specific needs but also makes it difficult to establish a standardised definition. Moreover, the evolving nature of technology and its applications is also contributing to the complexity of defining digital twins. As technologies advance and new possibilities emerge, the concept of digital twins may continue to evolve, making it challenging to pin down a static and universally applicable definition. In this sense it is important for stakeholders, researchers and practitioners to collaborate and share insights to develop a more standardised understanding of digital twins, even as the technology continues to evolve and find new applications.

In any case, the seamless incorporation of digitalisation approaches in the whole battery value chain holds the promise of significantly reducing the overall costs of battery cells. However, there are several challenges that must be addressed to move towards the digitalisation:

- First, while sensors and actuators play a crucial role in enhancing the quality of produced batteries and monitoring the production process, their current use is mainly limited to basic safety functions and defect detection. There is a need to explore and develop research activities focused on integrating intelligent sensors into existing production and testing facilities, enabling manufacturers and researchers to adopt agile methodologies and make real-time changes to processes and tests that can enhance battery cell performance.
- Second, the interaction between physical components and the virtual data layer of the real asset must be integrated efficiently. This involves considering technologies for data acquisition, storage and processing to enable the prediction of the impact of production changes on battery component structure and final cell performance.
- Furthermore, the vast and heterogeneous data generated in any point of the battery value chain poses a challenge for data storage, processing, and interoperability. Tools to support the



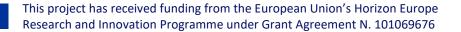
interoperability of battery manufacturing data and models used in digital twins are essential for seamless integration and simulation across different processes and equipment.

- Lessons learned from other industries, such as automotive and machining sectors, should be implemented in the battery field to encourage the use of common languages, interfaces, and protocols. In this sense standardised communication protocols and intelligent sensor systems will facilitate data use and exchange.
- Certainly, a crucial aspect in leveraging digital models as diagnostic tools and decision-making support tools lies in defining clear interactions and information exchange between different types of models, including high fidelity and low fidelity models. This necessitates the selection of suitable strategies for coupling and synchronizing these models, which presents a new challenge in achieving the aim of digital models effectively highlighting real-world circumstances.

All in all, overcoming the challenges associated with digitalisation in battery value chain will lead to the creation of a truly connected and intelligent environment. In such a scenario, the digital twin will play a pivotal role by accurately replicating physical assets and processes in the digital realm. This virtual representation will enable more effective monitoring, optimisation, and prediction of the corresponding physical battery chain throughout its lifecycle.

6.4 SoX monitoring

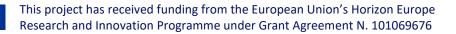
The implementation of SoX monitoring tools represents a crucial advancement in the field of battery management. The integration of real-time SoH, SoC, SoE, SoP, and SoS digital monitoring, facilitated by innovative physics-based and data-driven approaches embedded into digital twin frameworks, offers a comprehensive solution for the challenges posed by dynamic operating conditions and varying states of charge. As LIBs continue to dominate energy storage in commercial, industrial, and EV applications, harnessing the power of SoX monitoring tools into *intelligent* BMS is essential for unlocking their full potential, ensuring safety, and ushering in a new era of efficient and sustainable energy utilisation. Overall, employing intelligent BMSs for safe operation and optimal lifespan, coupled with an appropriate battery model, enables optimisation in battery design and use, including battery operating system components such as thermal management systems, protections, and electric drivers.



- Enhancing data acquisition and analysis: To improve accuracy and reliability in battery assessment, consider investing in robust data acquisition systems and analysis tools. This will enable more precise Coulomb counting and model-based estimation, leading to better decision-making regarding battery management.
- Integration of machine learning techniques: Explore the integration of machine learning techniques into data-driven methods for battery estimation. This could involve developing or utilising advanced algorithms to extract insights from complex data sets, thus enhancing flexibility and adaptability in battery assessment.
- **Continuous monitoring and optimisation**: Implement continuous monitoring of battery performance and condition, coupled with real-time optimisation strategies. Intelligent BMS systems can play a crucial role here by dynamically adjusting operational parameters to maximise safety and lifespan while meeting performance requirements.
- **Investment in battery modelling research**: Allocate resources towards research and development in battery modelling to refine existing models and develop new ones. This will contribute to more accurate predictions and optimisations in battery design and utilisation, especially concerning thermal management and protection systems.
- **Collaboration with battery manufacturers**: Foster collaboration with battery manufacturers to access detailed data and insights into battery behaviour and characteristics. This partnership can facilitate the development of tailored estimation methods and optimisation strategies aligned with specific battery chemistries and designs.
- **Cybersecurity aspects**: Cybersecurity at the hardware level is becoming increasingly important in today's interconnected world. With the rise of cyber threats and attacks, it is essential to take conscience and ensure the safety and privacy. By adhering to the regulations and guidelines set forth by the EU and other cybersecurity agencies, battery manufacturers can help mitigate risks and build trust. Ultimately, cybersecurity at the hardware level is not just a requirement, but a crucial component of building a secure and resilient intelligent BMS.
- **Regular training and skill development**: Ensure that personnel involved in battery assessment and management receive regular training and skill development opportunities. This will empower them to effectively utilise the chosen assessment methods and adapt to evolving technologies and best practices in battery management.

6.5 General remarks on digitalisation

The process of digital transformation frequently challenges organizations to venture beyond their familiar territories, compelling them to make strategic decisions for an uncertain future. In this context, the following actions are recommended to foster digital awareness within organisations undergoing digital transformation:



- Begin with **small-scale initiatives**.
- Participate in **standardisation** efforts.
- Assume responsibility for data ownership and ethics.
- Drive the change process and secure organizational commitment on the **digital transformation**.

7. REFERENCES

1 The European Green deal. European Commission Available at: <u>https://commission.europa.eu/strategy-and-policy/priorities-2019-2024/european-green-deal_en</u>. (Accessed: 24th April 2024)

2 Lex - 52022DC0552 - en - EUR-lex. EUR Available at: <u>https://eur-</u> <u>lex.europa.eu/legalcontent/EN/TXT/?uri=CELEX%3A52022DC0552&qid=1666369684560</u>. (Accessed: 24th April 2024)

3 https://batterieseurope.eu/wp-content/uploads/2022/09/Digitalization-Task-Force-Position-Paper 0.pdf

4 Stier, S. P., Xu, X., Gold, L. & Möckel, M. Ontology-Based Battery Production Dataspace and Its Interweaving with Artificial Intelligence-Empowered Data Analytics. Energy Tech; 10.1002/ente.202301305 (2024).

5 https://kiprobatt.de/wiki/Main_Page

6 https://www.celest.de/en/or/layer1

7 Clark, S. et al. Toward a Unified Description of Battery Data. Advanced Energy Materials 12; 10.1002/aenm.202102702 (2022).

8 Stier, S. & Gold, L. Battery Value Chain Ontology (BVCO) (Zenodo, 2024).

9 https://github.com/OO-LD/schema

10 https://catena-x.net/en/

11 https://www.big-map.eu/key-findings/battinfo

12 https://github.com/Battery-Value-Chain-Ontology/ontology

13 https://nexus.openIca.org/database/Environmental%20Footprints

14 Bhowmik, A. et al. A perspective on inverse design of battery interphases using multi-scale modelling, experiments and generative deep learning. Energy Storage Materials 21, 446–456; 10.1016/j.ensm.2019.06.011 (2019).

15 Benayad, A. et al. High-Throughput Experimentation and Computational Freeway Lanes for Accelerated Battery Electrolyte and Interface Development Research. Advanced Energy Materials 12; 10.1002/aenm.202102678 (2022).

16 Amici, J. et al. A Roadmap for Transforming Research to Invent the Batteries of the Future Designed within the European Large Scale Research Initiative BATTERY 2030+. Advanced Energy Materials 12; 10.1002/aenm.202102785 (2022).

17 Ling, C. A review of the recent progress in battery informatics. npj Comput Mater 8; 10.1038/s41524-022-00713-x (2022).



18 Green, M. L. et al. Fulfilling the promise of the materials genome initiative with high-throughput experimental methodologies. Applied Physics Reviews 4; 10.1063/1.4977487 (2017).

19 Deng, Z. et al. Towards autonomous high-throughput multiscale modelling of battery interfaces. Energy Environ. Sci. 15, 579–594; 10.1039/d1ee02324a (2022).

20 Bonilla, M. R., García Daza, F. A., Fernández-Pendás, M., Carrasco, J. & Akhmatskaya, E. Multiscale Modelling and Simulation of Advanced Battery Materials. In Progress in Industrial Mathematics: Success Stories, edited by M. Cruz, C. Parés & P. Quintela (Springer International Publishing, Cham, 2021), Vol. 5, pp. 69–113.

21 Franco, A. A. et al. Boosting Rechargeable Batteries R&D by Multiscale Modelling: Myth or Reality? Chemical reviews 119, 4569–4627; 10.1021/acs.chemrev.8b00239 (2019).

22 Danmarks Tekniske Universitet. Battery Interface Genome - Materials Acceleration Platform (BIG-MAP) [Grant Agreement No. 957189]. European Commission - CORDIS, 2022.

23 Uppsala Universitet. BATTERY 2030+: Coordination of large-scale initiative on future battery technologies (Batteries Partnership) [Grant Agreement No. 101104022, Fact sheet]1. European Commission - CORDIS, 2021.

24 Universidad Autónoma de Madrid. Development of Operando Techniques and Multiscale Modelling to Face the Zero-Excess Solid-State Battery Challenge (OPERA) [Grant Agreement No. 101103873, Fact sheet]. European Commission - CORDIS, 2023.

25 McCalla, E. Semiautomated Experiments to Accelerate the Design of Advanced Battery Materials: Combining Speed, Low Cost, and Adaptability. ACS engineering Au 3, 391–402; 10.1021/acsengineeringau.3c00037 (2023).

26 Flores-Leonar, M. M. et al. Materials Acceleration Platforms: On the way to autonomous experimentation. Current Opinion in Green and Sustainable Chemistry 25, 100370; 10.1016/j.cogsc.2020.100370 (2020).

27 Lombardo, T. et al. Artificial Intelligence Applied to Battery Research: Hype or Reality? Chemical reviews 122, 10899–10969; 10.1021/acs.chemrev.1c00108 (2022).

28 Stier, S. et al. The Significance of Accelerated Discovery of Advanced Materials to address Societal Challenges, 2023.

- 29 https://www.comsol.com/
- 30 https://www.ansys.com/products/fluids/ansys-fluent
- 31 https://pybamm.org/
- 32 https://batterymodel.com/battmo/
- 33 https://github.com/cidetec-energy-storage/cideMOD
- 34 https://www.acccellbat.eu/



35 https://thorbatteries.eu/

36 https://fastestproject.eu/

37 https://digibattproject.eu/

38 Shafto, M. et al. Modelling, Simulation, Information Technology & Processing Roadmap: Technology Area 11 (DRAFT).

39 Rosen, R., Wichert, G. von, Lo, G. & Bettenhausen, K. D. About The Importance of Autonomy and Digital Twins for the Future of Manufacturing. IFAC-PapersOnLine 48, 567–572; 10.1016/j.ifacol.2015.06.141 (2015).

40 Edström, K. et al. Editorial to the Special Issue: How to Reinvent the Ways to Invent the Batteries of the Future – the Battery 2030+ Large-Scale Research Initiative Roadmap (Adv. Energy Mater. 17/2022). Advanced Energy Materials 12; 10.1002/aenm.202270068 (2022).

41 Kies, A. D., Krauß, J., Schmetz, A., Schmitt, R. H. & Brecher, C. Interaction of Digital Twins in a Sustainable Battery Cell Production. Procedia CIRP 107, 1216–1220; 10.1016/j.procir.2022.05.134 (2022).

42 Kampker, A. et al. Concept for Digital Product Twins in Battery Cell Production. WEVJ 14, 108; 10.3390/wevj14040108 (2023).

43 Wang, W., Wang, J., Tian, J., Lu, J. & Xiong, R. Application of Digital Twin in Smart Battery Management Systems. Chin. J. Mech. Eng. 34; 10.1186/s10033-021-00577-0 (2021).

44 Wu, B., Widanage, W. D., Yang, S. & Liu, X. Battery digital twins: Perspectives on the fusion of models, data and artificial intelligence for smart battery management systems. Energy and Al 1, 100016; 10.1016/j.egyai.2020.100016 (2020).

45 Li, W. et al. Digital twin for battery systems: Cloud battery management system with online stateof-charge and state-of-health estimation. Journal of Energy Storage 30, 101557; 10.1016/j.est.2020.101557 (2020).

46 Naseri, F. et al. Digital twin of electric vehicle battery systems: Comprehensive review of the use cases, requirements, and platforms. Renewable and Sustainable Energy Reviews 179, 113280; 10.1016/j.rser.2023.113280 (2023).

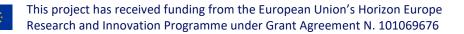
47 Zhang, R. et al. State of the Art of Lithium-Ion Battery SOC Estimation for Electrical Vehicles. Energies 11, 1820; 10.3390/en11071820 (2018).

48 Ungurean, L., Cârstoiu, G., Micea, M. V. & Groza, V. Battery state of health estimation: a structured review of models, methods and commercial devices. Int. J. Energy Res. 41, 151–181; 10.1002/er.3598 (2017).

49 https://catena-x.net/en/

50 https://www.big-map.eu/key-findings/battinfo

51 https://github.com/Battery-Value-Chain-Ontology/ontology





Contact us

www.batterieseurope.eu info@batterieseurope.eu